LITHIUM-CATION CONDUCTIVITY OF THE $LiMnPO_4$ SINGLE CRYSTAL

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Lithium-ion batteries are ones of the main technologies of energy storage, which play an increasingly important social role, in particular, because of their high capacity of energy. Lithium orthophosphates of the Li*M*PO_4 type (*M* = Fe, Ni, Co, Mn) show high electrochemical characteristics, which makes them attractive for use as electrodes. The other remarkable property of the Li*M*PO_4 orthophosphates with *M* = Fe, Ni, Co, Mn is the multiferroicity, i.e. a ferroelectric polarization and a long magnetic order are simultaneously present in these materials.

The aim of this work is to investigate the Li-ion conductivity mechanism by studying the crystal structure of the $LiMnPO_4$ single crystal using X-ray diffraction. At the same time our research focuses on the mechanism of a strong interaction between the ferroelectric and magnetic orders.

A single crystal of the $LiMnPO_4$ orthophosphate has been synthesized by a conventional solution growth in a LiCl flux. X-ray diffraction scans were carried out at the room temperature using the Rigaku XtaLAB P200 diffractometer (X-ray source Mo λ = 0.71073 Å, 2D detector (HPAD)) at the Seoul National University. To obtain the Li-ion migration maps (i.e. sets of migration paths of mobile cation within the framework) from crystallographic data implemented into the program package TOPOS [1].

Detailed X-ray diffraction study of the crystal structure and migration maps for single crystals of $LiMnPO_4$ orthophosphate have been carried out. The crystal structure of $LiMnPO_4$ consists of chains of edge-sharing MnO_6 octahedra and PO_4 tetrahedra which are connected by common edges O3-O3, between them there are tunnels of lithium octahedra along the *b*-axis. Their lattice constants, ion coordinates, anisotropic thermal coefficients, and occupation coefficients at the room temperature are specified. In the $LiMnPO_4$ orthophosphate lattice, the lithium ions migrate along channels oriented in the [010] direction, the ionic conductivity is anisotropic.

1. Blatov V.A. Multipurpose crystallochemical analysis with the program package TOPOS // IUCr CompComm Newslett. 2006. V. 7. P. 4.